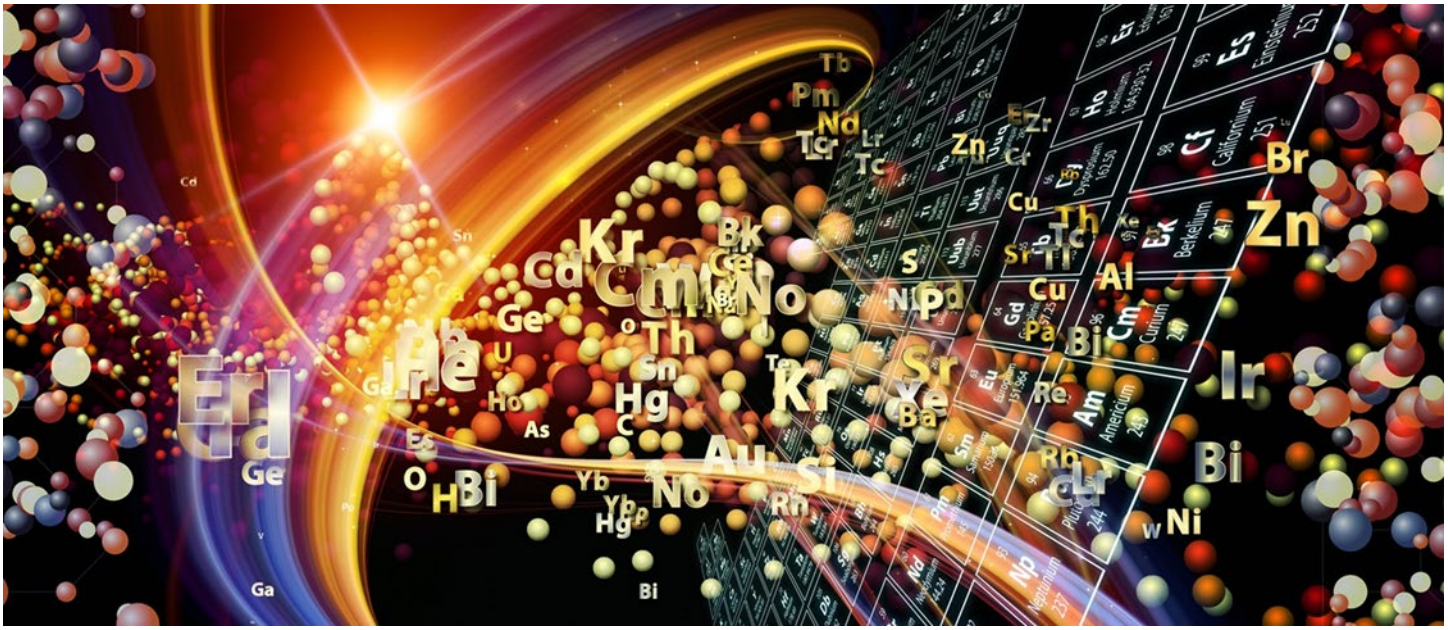

OLI Software Release Notes V9.6

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4/29/19

Contents

Introduction

For many years the OLI software release notes were maintained on several different web pages. While this was suitable at the time it has become far too cumbersome to maintain.

With the release of OLI Software V9.6 the release notes have been combined into a single document.

Each version will be listed in reverse chronological order. Within each version update to the products will be listed in this order:

- Databank updates
- Databank fixes
- Engine/solver
- OLI Studio/Analyzer
- OLI Flowsheet: ESP
- OLI Chemistry Wizard
- OLI Developer Edition
- OLI Alliance products
    - Aspen Hysys
    - Aspen Plus
    - gProms
    - IDEAS
    - ProII
    - Unisim Design
- OLI Security/License Manager

Version 9.6.3

General Information

The databanks were released on the same date as the first product. All engine/solver updates were included on the same date as the first release.

Product	Release Date
OLI Studio/Analyzer	May 1, 2019
OLI Flowsheet: ESP / ESP FS[1]	May 1, 2019
ESP Original	November 28, 2018[2]
Chemistry Wizard	May 1, 2019
OLI Developer Edition	May 1, 2019
OLI Engine 9.6 for Aspen Hysys	May 1, 2019
OLI Engine 9.6 for Aspen Plus	May 1, 2019
OLI Engine 9.6 for gProms	Not Released
OLI Engine 9.6 for IDEAS	Not Released
OLI Engine 9.6 for ProII	May 1, 2019
OLI Engine 9.6 for Unisim Design	May 1, 2019
OLI License Manager[3]	November 28, 2018

[1] The product ESP FS is for Asia releases. It is functionally identical to OLI Flowsheet: ESP.
[2] This is the absolutely final release of the ESP-Original product. There have been no updates to the user interface, only to the underlying engine.
[3] This product does not follow the same versioning scheme as the other products. The current version is 3.6.1.1.

Databank Updates

MSE model

There were no updates to the MSE databanks for version 9.6.3

MSE-SRK model

Revised systems

The molar volumes of all the n-alkanes were regressed v. carbon number to obtain a correlation for the Helgeson a_1 parameter in the equation of state. This was missing in the previous version. These a_x terms are important as the pressure increases and will shift the equilibrium constants for the Vapor-liquid1-liquid2 equilibria.

AQ model

There was no update for the AQ model for version 9.6.3

Engine/Solver/ESP Original

Bug ID	AREA	Problem	Resolution
791	Solver	**MSE-SRK L2 calculates inconsistently between points**	Solver strongly depends on initialization results, which cannot calculate any 2nd liquid if initialization suggests no 2nd liquid. In the initialization routine, there are several places to remove 2nd liquid if optimization is stuck. Those criteria are changed to allow finding 2nd liquid. VLE_SOLVE is also used to estimate V/L2 amount for a new initial guess for some cases. After the changes, MSE and MSE-SRK can solve 2nd liquid for all temperatures in the reported file. This also solves Jim's file of Hg vapor pressures, which is caused by the 2nd liquid not appearing continuous. However, computational time is observed to increase, which will be quantified in the following test case validation.
814	Solver	**This case has a temperature survey. In the area of about 70 C, there is a break in the curve where everything goes into the vapor phase. Yet slightly above that temperature or below that temperature the curves seem correct.**	At 70 C, the initialization process quit at ITACT=3 and solver didn't find solution with such bad initialization. The criteria for initialization keep iterating is ITACT < 3 or SNORM <5. Changed to ITACT < 4 or SNORM <5 solved this problem. The possible cost would be for other cases with such bad initialization iterations, engine will take one more activity (120 iterations) before moving to next step. The increased time should not be noticeable.
910	Engine	**Implement new Pseudo Component interactions for MSE-SRK**	Parameters updated for new interactions.
933	Solver	**A user found an issue which he shows below. It can be summarized. Using discrete organic components in MSE-SRK he gets a reasonable organic solubility in a brine. Using pseudo-components, he gets a different solubility for the same components' molecular weights.** **There is also a funny spike is when NaCl forms as a solid and drops out of solution. This occurs in the vicinity of 200 atmospheres.** **The user is concerned that his phase flow predictions are off because of the pseudo components.**	The parameters updated along with solver updates in Bug ID's 791 and 910 resolved this issue.

OLI Studio/Analyzer

There were no interface updates to OLI Studio/Analyzer.

OLI Flowsheet: ESP / ESP-FS

There were no interface updates to OLI Flowsheet: ESP / ESP-FS.

Alliance Products

There were no interface updates to OLI Engine in any Alliance products.

Version 9.6.2

General Information

The databanks were released on the same date as the first product. All engine/solver updates were included on the same date as the first release.

Product	Release Date
OLI Studio/Analyzer	November 28, 2018
OLI Flowsheet: ESP / ESP FS[4]	November 28, 2018
ESP Original	November 28, 2018[5]
Chemistry Wizard	November 28, 2018
OLI Developer Edition	November 28, 2018
OLI Engine 9.6 for Aspen Hysys	November 28, 2018
OLI Engine 9.6 for Aspen Plus	November 28, 2018
OLI Engine 9.6 for gProms	Not Released
OLI Engine 9.6 for IDEAS	Not Released
OLI Engine 9.6 for ProII	November 28, 2018
OLI Engine 9.6 for Unisim Design	November 28, 2018
OLI License Manager[6]	November 28, 2018

[4] The product ESP FS is for Asia releases. It is functionally identical to OLI Flowsheet: ESP.
[5] This is the absolutely final release of the ESP-Original product. There have been no updated to the user interface, only to the underlying engine.
[6] This product does not follow the same versioning scheme as the other products. The current version is 3.6.1.1.

Databank Updates

MSE model

There was no update for the MSE databanks for version 9.6.3

MSE-SRK model

Revised systems

Densities of hydrocarbons

Densities of pseudocomponents

AQ model

Name, synonym, and mineral name corrections

Cyanide ion

Triethanolamine

Methanol

Triacontane

Methyl isobutyl ketone

Thiosulfate ion

Dithionate ion

Databank fixes

Bug Number	Description
3703	Synonym data for TEXH is the same as for TEXH2CL
3806	MSE: IUPAC name (display name) for methanolate ion does not have a charge
3905	IUPAC name for TRICONTAN is incorrect
3978	Add Synonym for methyl isobutyl ketone (MIBK)
4078	IUPAC for S2O3ION and S2O4ION seems to be incorrect.
4367	methanolate ion named as ethanolate ion in MSE
4603	MSEPUB: no mineral name for a species that is a sodium aluminiosiliate gel
4924	Synonym for methanol should be CH3OH
OS-439	MBG name for cyanide is Cn(-1) but should be CN(-1)
OS-418	Two liquid phases formed when NdPO4 is added in H3PO4+H2O mixtures at 25C, 1atm; very unreasonable 2nd liquid phase composition (“ionic liquid” like)

Engine/Solver/ESP Original

Bug ID	AREA	Problem	Resolution
OS-404	Solver	Crash in flashing the Liquid 2 only stream	Liquid-2 only stream accesses the output array for T&P before density calculation and those are not stored in the array initially. Updated the checks to verify if the pointers exist.
OS-411	ESP	ESP original does not have the MSE-SRK option	This will not be implemented. If the user requires ESP Original with MSE-SRK the Chemistry Wizard can be used.
OS-429	Solver	LLE calculation fails when using MSE-SRK and no hydrocarbons are involved	Adjustments have been made to LLE calculations in MSE-SRK that eliminate this problem. However, through testing of this improvement is needed.
OS-477	Solver	AJ has reported this case. The final scaling object will fail to converge if Rigorous pre-scales are enabled or no pre-scales are enabled. If estimated pre-scales are enabled the case will converge.	There is no resolution for this case. It requires an update to the FORTRAN compiler not scheduled until V10 of the of the software
OS-509	Solver	Crash in surface complexation without water	The crash was stopped by checking if the molality is greater than zero. There were multiple checks added in surface complexation algorithm to avoid divide by zero.
OS-522	Solver	Crash in Surface complexation with 2nd liquid phase. If 2nd liquid phase is turned off, calculation runs fine.	The crash happens the perturbative jacobian calculation routine in the initializer. It appears the initializer allows for surface species(CPM and CPI) to be allowed in the 2nd Liquid. But on checking the code always the number of unknowns are one more than the number of equations. This is because the AQ-ORG equation only adds equations with species corresponding to AQ suffix. CPM (uncharged)suffix was added and the number of equations match the number of unknowns.
OS-547	Solver	Calculated density of Assay is Different in all three different frameworks	The pseudo-component fractions in the assay are heavy boiling fluids • MSE-SRK uses the volume translated SRK method to determine the density of the mixture. No volume translation parameters have been developed for pseudo-components, hence the density contribution is solely from SRK resulting in significant deviation from API calculated assay density • AQ model uses the Rackett equation for calculating density hence differing from API • MSE uses the HKF (can have volume translation contributing if parameters exist) plus excess for calculating volume. This is closest to that reported by API Volume translation parameter correlation was developed for Pseudo components.
OS-568	Solver	Remove special code for NH4OH as solvent for certain transport properties	Code Removed and tested. Same results obtained as in 9.5.4.

OLI Studio/Analyzer

Bug ID	AREA	Problem	Resolution
OS-31	Stream Analyzer	Phase Envelope calculation has different results with different starting and ending temperatures	The Upper bound for pressure in the dewpoint curve was fixed by the maximum attainable pressure obtained from the bubble point curve. This was fixed by allowing the dewpoint curve calculation to compute 2% above the bubble-point max pressure if the equilibrium calculation succeeded at every previous iteration after this maximum was reached. In the survey (0-900 x 2.5), the Temperature range was outside the bubble-point curve computation, thus allowing dewpoint curve to go unbounded and hence completing the curve The algorithm has significant room for improvement in terms of speed as well as obtaining the full curve more consistently.
OS-49	User Interface	Report total dissolved silica as SiO_2 instead of using the MBG groups.	Implemented framework to calculate and report common representations such as 'Total Si as SiO2' and 'Total P as PO4(-3)'. The framework is implemented in a common layer that both Flowsheet: ESP and OLI Studio can use.
OS-50	User Interface	Report surface complexes as adsorbed species	Adsorbed is displayed as "Surface Species" in output grids and reports. Adsorbed is still considered as part of the solid phase so if user turns off the solid phase on the report session the Surface Species will be hidden as well. On the other hand, if no adsorbed is formed the reports won't show Surface Species column even solid phase is turned on and solid species exist. All the adsorbed species are removed from the solid species array; i.e. a solid species can exist in either the solids or the adsorbed, but not both. Code is not checked in yet. Screenshots have been uploaded here for review.
OS-78	Units Manager	Adjust the units selection list to have the gauge pressure units right after the corresponding base unit	Reordered units so “Gauge” units appear alongside absolute units.
OS-80	Stream Analyzer	These are feature and actions requests for the new "Volume units in Stream Amount" function that was added in V9.2.7. 1) Default is Fixed condition 2) Default Conditions 25C, 1 atm	Items 1 and 2 are implemented
OS-99	Stream Analyzer	Please enable the Calculation type option when doing a pH survey.	FixFree (Custom) is now one of the SuveryCalcTypes. User can assign pairs of fixed/freed variables (parameters or species), and select one fixed to survey. This is an alternative to the original request "Enable calculation type in pH survey", and it should work more flexible as pH is not the only variable can be surveyed.
OS-100	ScaleChem	Add the solids PbS and ZnS the standard list of solids.	PbS and ZnS are now in the standard solid list (Scenario, Saturator, Mixing Water, Facilities). If either PbS or ZnS are in the model, it will be displayed in the standard solid section of the list.
OS-196	Stream Analyzer	Turn off Calculation Summary in report as a default.	Calculation Summary and Stream Inflows in the report are now turned off by default (Single Point and Survey). However, Calculation Summary will not be turned off for the Mixer. This is fixed and checked in.

Bug ID	AREA	Problem	Resolution
OS-268	Stream Analyzer	This story is derived from an embarrassing situation. The NACE TG299 round-robin teams used the AQ-FWK and Stream Analyzer objects to predict an oilfield condition of 1400 bar. Unfortunately, the T/P span for Stream Analyzer objects extend to 200 bar, and the results obtained by some of the teams included a 4.1 pH while others using AQFW in ScaleChem computed a 5.2 pH. It is worth discussing if it is still necessary to have this T/P span selected for Stream Analyzer objects and if so, might we increase this to the 1500 bar that is defaulted for ScaleChem. We can discuss the potential drawbacks, and if no change can be made here, then perhaps we can provide warnings when the conditions tested extend beyond the T/P Span.	We have studied the effect of increasing the T/P span (as in ScaleChem objects) for Stream Analyzer objects. The objective was to investigate how the increased T/P span changes the predictions not only at higher temperatures and pressures but also within the default. The analysis was conducted as described below: (1) Increased T/P span and checked effect on our standard cases: K values were insignificantly different, initialization was different for few cases, but little to no change in final results. (2) Increased T/P span and checked effect on our standard corrosion cases: Corrosion rates were different but remained within the experimental error. (3) Increased T/P span and crosschecked with validation cases (provided by the data team), cases were for high pressures (up to 1500 atm) and moderate temperatures (up to 300 C). System include BaSO4, BaSO4 + NaCl, BaSO4 + CaCl2, BaSO4 + MgCl2 and such. Overall, not significant divergence in the predictions were found and increasing T/P span did not compromise the fit in the default T/P range as seen in the aforementioned cases.
OS-362	ScaleChem	Add partial pressures and fugacity values to ScaleChem Reports	Values added to reports.
OS-364	PIPESIM PVT File	Error message from PVT file "The PVT file location specified is invalid."	There are 2 issues here. The filename was limited to 132 characters for no reason other than an arbitrary number being used in the code. Changed to be dynamic to the size of the filename supplied. The initial file name is based off the object name and object names can have characters that are not acceptable for filenames. Added code to update the filename and remove the bad characters when first creating the name.
OS-365	PIPESIM PVT File	While working on case OS-364 the PVT file fails near the end of the run. All the results are then removed. So, there is really two issues. The convergence failure with the message and the loss of data.	Updated code to display errors for interpolation but results for contour plot are retained. Also updated error messaged to show they are related to PVT generation
OS-370	Stream Analyzer	Calculation options icon in the Tool bar doesn't have a Tool Tip	Added tool tip for calculation options button.
OS-371	Stream Analyzer	Tool tip in MSE-SRK button should say: Use MSE-SRK Databanks	Updated tooltip to display MSE-SRK also updated status bar message to show MSE-SRK.
OS-373	Engine	In a dual survey in Temp and Press. All is ok until the Liq2 phase appears. We mistakenly report a vapor phase fugacity when the value should be zero. This is a pure component, it can be either a liquid or a gas but not both unless at the boiling point. We incorrectly copy over the fugacity coefficient.	Incorrect use of memory duplicated values when zeros were detected.
OS-389	Engine	Should not report fugacity coefficient for a component with zero inflow	Fugacity is not reported for components with zero flow.
OS-391	ScaleChem	Case runs for a long time, but trace file indicates it has converged	New TDS calculation can hang up and take a long time to run. There is not an error here.
OS-408	Calculation	Precipitation point calculation crashes in Studio with MSE 2nd liquid turned on. Calculates OK with 2nd liquid turned off.	This needs to be tested with the updated databank. A check was added not to remove the target species from equation.

Bug ID	AREA	Problem	Resolution
OS-405	Stream Analyzer	Calculate a calcObject may clear the results of another calcObject	This is due to CalcObj not updating parent Stream's Chemistry Model if their Chemistry Models are different, e.g. Parent Stream using Aq and CalcObj using MSE. It is now fixed by making sure Parent Stream's Chemistry Model is up to date when calculating the CalcObj. Code has been checked in.
OS-410	Chemistry Model	Switching the thermodynamic framework from MSE with UREA databank selected to MSE-SRK does not hold the UREA databank selection. Corrosion, Geochemical, Surface complexation hold.	Updated cross-reference list to allow UREA databank to stay selected between MSE & MSE-SRK
OS-412	Data Locator	Does not support MSE-SRK	Support for MSE-SRK added.
OS-429	Engine	LLE calculation fails when using MSE-SRK and no hydrocarbons are involved	Adjustments have been made to LLE calculations in MSE-SRK that eliminate this problem. However, through testing of this improvement is needed.
OS-439	Database	MBG name for cyanide is Cn(-1) but should be CN(-1)	Name updated by Data Team
OS-452	Database	Imported Database has incorrect interaction parameters. ESP format database in local directory is correct, copied database in store folder is incorrect.	The issue could be in cpp based ascii files writer. The writer puts the decimal from the last entry to a new line and subsequently the decimal becomes a new entry and ignores the next number.
OS-454	All Products	Change the default P-Span from 1 - 201 atm to 1 - 1500 atm in all products.	Updated default P-Span for OLI Studio. With the same caveat as OLI Flowsheet:ESP old cases will retain the previous setting. Also since the default is saved in preferences clients that have 9.6.1 installed already will need to reset the defaults in order to have the new range applied. Also now going to display the ranges all the time in the summary window not just when overridden.
OS-456	Calculations	Calculation fails when copying and pasting streams in autoclave	Updated validation logic to validate the gases and display an error to the user when one or more of the specified gases are not in the model. This is what was occurring in this case, one of the gases was added at the calculation level and was not in the pasted calculation due to the current shortfall in copy/paste.
OS-459	Engine, ScaleChem	The problem is that when using MSE-SRK and H2O saturation calculation, the oil analysis is predicted as all vapor. AQ and MSE predict it as L2.	Engine keeps track of initialization failure but uses some earlier results to reinitialize. Added code to check if the used results are valid for subsequent re-initialization context.
OS-464	Stream Analyzer	Solids indicated by Scale Index not the same as Scaling Tendency	Lists now based on Scale Tendency values
OS-467	ScaleChem	Please add a pop-up or other appropriate warning that communicates to the user that the Phase Type they selected (gas or oil) has a zero-phase amount. This is because the calculated mass rate of that inflow stream will be zero if that phase fraction is zero. This again, is because the inflow rate selected is based on a specific phase (gas or oil type).	Any inlet requesting Oil or Gas phase ends up getting 0.0 amount will fail the calculation. Code has been checked in.
OS-478	ScaleChem	A user responded below, and he did not follow-up with complaints about the Saturation results. His remaining concerns are derived from the odd fluid composition and not anything that the software created. The saturation option should be deactivated until we have a new design or until we add some safety precautions.	Added an app-wide preference (accessible under the 'Advanced' subheading in the 'General' tab of the Tools->Options UI) to enable/disable 'Saturate With' option in the specs UI for oil or gas analysis objects.

Bug ID	AREA	Problem	Resolution
OS-486	ScaleChem	When using MSESRK, the pre-scale tendencies are exactly 1. If we switch to rigorous, then the actual values appear in the table.	Prior to the call to the phase estimation routine, the pre-scaling index array may be cleared. The phase estimation routine does not check if the arrays are zeroed out and overwrites with the current value of the scaling index. Check was added if the pre-scales have been calculated.
OS-487	Autoclave	Unable to delete pressure entry in Autoclave when using psig	Currently, the pressure is stored in atmospheres so when a 0 value for psig is entered it is converted to atm and then back again. This results in -1.77636e-15 psig not 0. This causes the deletion logic to fail. I have adjusted the logic so that pressing the delete key will clear the pressure entries in Autoclave. However, entering a value of 0 psig will still result in the -1.77636e-15 psig showing for the pressure. I will clone this bug to address the conversion error separately.
OS-497	ScaleChem	Program terminates without any warning or error (possible unit conversion error)	The conversion for lb/1000bbl used in the scaling scenario report, did not consider the possibility of a user switching out of concentration units. When the units were not in a concentration basis this conversion was not possible as a simple conversion causing the error. Updated the code to always use a concentration-based unit set to show this value, also added code to protect against a crash in this case which will just leave the field blank.
OS-513	Stream Analyzer	The element reporting (Mat Codes/MBGs) need to have the surface species separated out. This involves the reports, plotting and the grid.	Surface species for MBG in reports, grids, and plots are implemented. We do not have room for a _fw enum and we did not add a new Phase::enum for surface species. The work around is surface species still use solid enum (both _fw and Phase) Stream and MaterialBalanceGroup classes have special code to recognize request from UI. Code has been checked in.
OS-525	Engine	In an MSE-SRK case which has no water. Apparently no equilibrium calculation has been done. However, all the material is reported as in the solid phase. This is an invalid condition and needs error handling or an equilibrium calculation should be attempted and then failed.	No water in MSE-SRK is a que for the program to try organic equilibrium using SRK. Since the components do not contain VAP species(NACL!), even the organic equilibrium fails, leaving only solids as viable option(both MEG and NACL have solid phases). The fix would be to try to push to solver since technically MEG + NACL is a valid MSE case(MEG in liquid 1 and NACL in solids), but the caveat is that no 2nd liquid can be formed in the system. What this means is that if you include another component that has a propensity to form a separate liquid phase the phase behavior will be unpredictable.
OS-543	User Interface	Disconnected stream has stray values in components that should be zero	There were issues with initializing and clearing some arrays. When stream input/inflow changes, based on the conditions solver takes different routes. Some earlier calculated values became irrelevant in that context. which needed to be cleared.
OS-544	Engine	Gas is appearing as a L2 when having assays in the inflows, even when L2 is turned off	Few issues were corrected in alternate VLE solver based on Rachford-Rice algorithm.
OS-545	User Interface	I wanted to check the warning error and identify the stream or block that is causing the warning, but it does not give enough information. When I go to the .wrn file, the information in parenthesis says: NULL NULL NULL.	Previously the warning description was only done for assay->pseudo-components work flow. Causing truncated warning messages to appear when only pseudo-components are in inflow Only cut number was shown before, now its replaced by names
OS-547	Engine	Calculated density of Assay is Different in all three different frameworks	The pseudo-component fractions in the assay are heavy boiling fluids MSE-SRK uses the volume translated SRK method to determine the density of the mixture. No volume translation parameters have been developed for pseudo-components, hence the density contribution is solely from SRK resulting in significant deviation from API calculated assay density AQ model uses the Rackett equation for calculating density hence differing from API MSE uses the HKF (can have volume translation contributing if parameters exist)+ excess for calculating volume. This is closest to that reported by API Volume translation parameter correlation needs to be developed for Pseudo components.

Bug ID	AREA	Problem	Resolution
OS-569	Stream Analyzer	If there is no surface species in the output stream, the "Surface Species" grid section should be hidden. When user right click on the output grid area it should not be on the pop-up menu list. Common Representation should have the same logic.	Resolved

OLI Flowsheet: ESP

Bug ID	AREA	Problem	Resolution
OS-34	User Interface	When changing a stream unit set, the callout units don't change.	Allowing a source block or stream unit change the callout table unit If a user changes the callout table unit, then the callout stops following the source object unit. If a user changes the source block or stream and callout unit at the same time, then the callout will follow the source unit change (Resetting)
OS-39	User Interface	When a controller is disabled, it should not be asking for the "Target Value". Currently, it shows error.	Corrected process validation code to skip checking for missing/unspecified specs in a disabled controller.
OS-42	User Interface	FEATURE: Add the ability to “Step” through a calculation block-by-block	Added support for stepping through a single block calculation. An overlay icon is displayed to indicate the paused block in flowsheet view.
OS-49	User Interface	Report total dissolved silica as SiO_2 instead of using the MBG groups.	Implemented framework to calculate and report common representations such as 'Total Si as SiO2' and 'Total P as PO4(-3)'. The framework is implemented in a common layer that both Flowsheet: ESP and OLI Studio can use.
OS-78	Units Manager	Adjust the units selection list to have the gauge pressure units right after the corresponding base unit	Reordered units so “Gauge” units appear alongside absolute units.
OS-230	User Interface	Customer is looking for named callout templates which are related to the unit operation for example: Downstream of an RO will have different template than downstream of a stripper. The callouts are defined by the user similar to plot template manager.	Added support for callout templates. Added a panel within the callout properties page that allows selection of an existing template or creation of a new one based on the current settings of the callout.
OS-279	Sensitivity	Analysis tool in Flowsheet, does not honor increment value	Fixed
OS-298	PFD	Customer is looking to add general annotations to flowsheet, we should allow text annotation, the drawing of lines and rectangles to the flowsheet. Also add the ability to add variable names for file names, path, etc.	• Add arrow, rectangle, text labels and bitmap on flow-sheet via toolbar • Allow to resize, move, delete annotation objects
OS-299	File Management	Can we get the File-Properties in during the beta. I want to see the version that clients are using when they send files. This would be similar to what OLI Studio current uses.	Added File "Properties..." option on the OLIFlowsheet "File" drop-down menu
OS-352	Unit Operations	FEATURE: Add isochoric mixing as an options for mixing unit operations.	Unit Operation added.
OS-369	User Interface	When opening a file saved with an older version we should save the file with the older version number displayed.	This was implemented for OLI Studio. See OS-310
OS-372	User Interface	Inlet stream flash composition changes when different chemistry model is selected for the block. Multiple chemistry model issues.	Added multiple chemistry model terminal error check which invalidates the case.
OS-395	Engine	RO membrane reports non-converged stream when it looks like everything is converged	Errors in the block (e.g., flash failure terminal messages) are selectively cleared from the error array if block passes.
OS-396	User Interface/Import	Importing an ESP-Original file with an incinerator unit operation fails	The structure of the new incinerator block is much different from the older version. No support is included since usage was very low.
OS-403	Engine	To help support Autoclaves we need to add partial pressure to a controller. This means having to first define it and then control it. We could also add Fugacity as well.	Added initial engine code for Partial Pressure & Liquid Fugacity in Controller options. For Partial Pressure, at the equilibrium composition, the species vapor pressure will we given as P_j = Y_i * P_total, where Y_i is the mole fraction of the species in vapor phase and P_total is the total pressure.

			For Fugacity, at the equilibrium composition, if vapor phase is present the algorithm will use the vapor phase species fugacity. If there is no vapor phase, it will use the liquid phase fugacity for that species for either liquid-1 or liquid-2. Preference is given to liquid-1. Fugacity for the liquid phase is given by the relation: Phi = exp((u_liquid - u_vapor) + R*T*(x_i*Gamma_i)) Phi = liquid phase fugacity u_liquid = standard state chemical potential(liquid species) u_vapor = standard state chemical potential(vapor species) R = Universal gas constant x_i = mole fraction (liquid species) Gamma_i = Activity coefficient (liquid species) of x_i User Interface Spec for Flowsheet: ESP Allow option for Partial Pressure and Fugacity (units of Pressure) in Controller "Spec. Type" This should bring up a drop-down option to choose a VAP species.
OS-409	User Interface/Tools	Molecular conversion user specified weight factor could be 1~100. Currently, it is 1~10.	Updated the range.
OS-416	User Interface/Reports	Please add the pre-scale tendencies to the list of calculations.	Added to calculations.
OS-421	User Interface/Tools	The way the user is informed that a restart is required if the private databank folder is changed is currently a static message on the screen that is always there. This needs to be a popup message that is displayed when the user hits the ok or apply button. If we change to applying the databank change dynamically this change would not be needed. Also, the screen refers to "database" and it should be databank as this is the term we consistently use in our products. The title should be Private databank location and the category tree should also be Databanks.	• Changed the display text on the databank option page • Added popup warning message
OS-423	User Interface	CRASH: Program crashes when clicking on the Chemistry Tab, uses private database	Improved fault tolerance of code that read data from databases that have data consistency errors.
OS-436	File operations	Specification of vapor species for controlling partial pressure or fugacity is lost when the file is reopened	Correctly save and load vapor species selection in controller's fugacities and partial pressures specification from the case file
OS-440	User Interface	I feel that we need to add a disclaimer saying that the simulation results are based on the OLI Technology. The Membrane specifications available in the library are merely used a basis for building the membrane in the simulation.	This was checked in. It was checked in to the ro_membrane thread, but Sachin already merged the thread to the main thread.
OS-444	Engine	Engine support for surface species total amounts	Engine work completed for surface species mole/mass/volume calculation. New EQSOLD (for stream analyzer) and EQBLKSOLD (for flowsheet) ID's have been established for surface complexation species total mole/mass/volume calculation:
OS-446	User Interface	Recently while working on a case with a customer, I was realized the need of this feature while demonstrating F_ESP capabilities to her. Our reactor block call-out contains only standard block information like heat duty, inlet mass, outlet mass. It's missing a section called	Added support for displaying calculated extent of a reaction along with its equation in a callout.

		Calculated Data, like we have for Separator. A user can benefit from a quick glance at what reaction took place and the extent of reaction (which is available in the standard block report for the reactor) in the call out.	
OS-447	User Interface	Incinerator exit temperature is an estimate and not a spec, should be so indicated	Added prefix "Estimate" to "Temperature" when using adiabatic calculation Merged "Parameters" section with "Equilibrium Calculation" section for simplicity
OS-457	Sensitivity	Plot of sensitivity analysis doesn't show the correct values	Fixed sensitivity analysis code that was losing composition amounts in monitored species when artificial kinetics species were present in the model.
OS-461	User Interface	FEATURE: I need the controller to adjust the Conversion Fraction in the Stoichiometric Conversion option of the reactor. In this way, the Client can adjust the amount of available MagOx surface based in the dissolved Silica (or borate) concentration in the clarifier overflow.	Added, see OS-494
OS-471	Sensitivity	Please find the attached file and plot image, I have pH on Y2 axis and the icon used for that plot has been repeated in the sensitivity analysis for HCl vapor on Y1 axis.	Fixed logic that sets up the default colors and symbols for curves to ensure that a color and symbol combination is not repeated.
OS-484	User Interface	The flowsheet callout tables and reports do not display the fugacity and partial pressure values This is needed if we are to deliver Autoclave in Flowsheet.	Values are now properly displayed in the callouts.
OS-494	User Interface	FEATURE: Please look into the feasibility of including CONV as a sensitivity variable for the reactor. Keep in mind that there may be multiple stoichiometric reactions in a given reactor and therefore more than one CONV variable.	Added support for specifying a stoichiometric reaction's conversion fraction as a sensitivity parameter and in a controller.
OS-495	Engine	The stream "Air" fails to converge. It should, it is just CO2, N2 and O2 at ambient conditions. The stream seems to get out of bounds. A crash is reported in the OUE file but that may be due to the non-convergence.	There were errors in surface species molality and volume calculation, which have been fixed. Even though there were no surface species inflow, but being in the chemistry model, it still needs to check for molality and volume for surface species.
OS-499	Batch Files	Validate ESPBAT.exe will work with OLI Flowsheet:ESP install and can be supported	ESPBAT.exe calls BLMAIN1 function, which is supervisory run function in blmain1.for in project ASAP. Call to dll version(BLMAIN_DLL) has been commented out, due to the fact that the project links to espf.lib making it a dependency for spreadsheet based calculations. Also keydll.dll has been configured to be delay-loaded, since its not installed with FESP. Tested with Tower case (ABSORB) in standard test sets. Case ran successfully in this mode espbat.exe can run from FESP root executable directory
OS-500	Surface Complexation	A case had a stream with a solid-only designation but using a surface complexation species such as CPM. This failed with no error messages	The CPM is actually an aqueous species and requires H2O to worked. These types of cases are trapped out and an error message displayed.
OS-501	Databanks	The way the user is informed that a restart is required if the private databank folder is changed is currently a static	Changed the display text on the databank option page Added popup warning message

		message on the screen that is always there. This needs to be a popup message that is displayed when the user hits the ok or apply button. If we change to applying the databank change dynamically this change would not be needed. Also, the screen refers to "database" and it should be databank as this is the term we consistently use in our products. The title should be Private databank location and the category tree should also be Databanks.	
OS-510	User Interface	Surface complexes not reported in MBG for Flowsheet	Species are now properly reported
OS-512	User Interface	Need to implement concentration units for "OS-49 Report total dissolved Silica"	OS-512: The concentration is implemented. All batch units (Mass and Mole concentration and fraction) are tested and passed. Code has been checked in.
OS-514	User Interface	The element reporting (Mat Codes/MBGs) need to have the surface species separated out for reports etc.	Added support for reporting MBG-totals for surface species separately from the solids. This is honored in all UIs including callouts and sensitivity plots.
OS-515	User Interface / Reports	Include a filter to exclude solids in the report which are outside their TRANGE	Added support for filtering out scaling tendencies that are out of Solid K-Fit TRange showing in single stream and multi-stream reports. Also added support for optionally displaying the TRange next to the solid species in the report. The report customization UI now shows additional TRange related options for scaling and pre-scaling tendency sections.
OS-516	User Interface / Reports	Na2SO4 appearing in Flowsheet ScaleTendency table when it is out of range	See OS-515 above

Alliance Products

Bug ID	Product	Problem	Resolution
OS-413	Aspen Hysys	MSE-SRK does not work in Aspen Hysys V10	HYSYS reads the databanks in the reverse order, starting with MSEPUB and then the private databanks. This caused MSE-SRK private databank to be invalidated since an additional check was added to see if MSEPUB was added at the end. Fixed by Changing the order of the databanks directly when HYSYS calls the OLIEngine
OS-482	Unisim, ProII	The OLI Data Locator program is not included in the installs	Added the product to ProII and Unisim Design installs for the OLI Engine.

Version 9.6.1

General Information

The databanks were released on the same date as the first product. All engine/solver updates were included on the same date as the first release.

Product	Release Date
OLI Studio/Analyzer	June 5, 2018
OLI Flowsheet: ESP	June 6, 2018
ESP Original	June 1, 2018
Chemistry Wizard	June 1, 2018
OLI Developer Edition	June 3, 2018
OLI Engine 9.6 for Aspen Hysys	June 14, 2018
OLI Engine 9.6 for Aspen Plus	June 14, 2018
OLI Engine 9.6 for gProms	Not Released
OLI Engine 9.6 for IDEAS	Not Released
OLI Engine 9.6 for ProII	June 14, 2018
OLI Engine 9.6 for Unisim Design	June 14, 2018
OLI License Manager[7]	Not Released

[7] This product does not follow the same versioning scheme as the other products. The current version is 3.4.3 released July 31, 2017

Databank Updates

Mixed-solvent electrolyte databanks:

MSEPUB

Potash systems

Binary system

$MgSO_4$ including (revised):

$MgSO_4 \cdot 12H_2O$	
$MgSO_4 \cdot 7H_2O$	(epsomite)
$MgSO_4 \cdot 6H_2O$	(hexahydrite)
$MgSO_4 \cdot 5H_2O$	(pentahydrite)
$MgSO_4 \cdot 4H_2O$	(starkeyite)
$MgSO_4 \cdot 1H_2O$	(kieserite)

Ternary systems

$MgSO_4 – MgCl_2$ (revised)

$MgSO_4 – K_2SO_4$ including double salts:

$K_2Mg(SO_4)_2 \cdot 6H_2O$	(schoenite, picromerite)
$K_2Mg(SO_4)_2 \cdot 4H_2O$	(leonite)
$K_2Mg_2(SO_4)_3$	(langbeinite)

$CaSO_4 – K_2SO_4$ including double salts (revised)

$K_2Ca(SO_4)_2 \cdot H_2O$	(syngenite)
$K_2Ca_5(SO_4)_6 \cdot H_2O$	(gorgeyite, pentasalt)

$MgSO_4 – Na_2SO_4$ including double salts

$Na_2SO_4 \cdot MgSO_4 \cdot 4H_2O$	(blödite)
$Na_2SO_4 \cdot MgSO_4 \cdot 2.5H_2O$	
$3Na_2SO_4 \cdot MgSO_4$	

$MgSO_4 – H_2SO_4$ including acid/double salts (revised)

$Mg(HSO_4)_2 \cdot 2H_2O$
$Mg(HSO_4)_2 \cdot 2H_2SO_4$

$CaSO_4 – MgSO_4$ (revised)

$CaSO_4 – MgCl_2$ (revised)

Quaternary systems

$Mg – K – Cl – SO_4$ including double/multiple salts:

$KMg(SO_4)Cl \cdot 3H_2O$	(kainite)

$KMgCl_3 \cdot 6H_2O$ (carnallite)
$K_2Mg(SO_4)_2 \cdot 6H_2O$ (schoenite, picromerite)
$K_2Mg(SO_4)_2 \cdot 4H_2O$ (leonite)
$K_2Mg_2(SO_4)_3$ (langbeinite)

Mg – Na – Cl – SO_4 including double/multiple salts:
$9Na_2SO_4 \cdot MgSO_4 \cdot NaCl$
$Na_2SO_4 \cdot MgSO_4 \cdot 4H_2O$ (blödite)
$Na_2SO_4 \cdot MgSO_4 \cdot 2.5H_2O$
$3Na_2SO_4 \cdot MgSO_4$

Mg – K – Ca – SO_4 including double/multiple salts:
$K_2Ca_2Mg(SO_4)_4 \cdot 2H_2O$ (polyhalite)
$K_2Ca(SO_4)_2 \cdot H_2O$ (syngenite)
$K_2Ca_5(SO_4)_6 \cdot H_2O$ (gorgyite, pentasalt)
$K_2Mg(SO_4)_2 \cdot 6H_2O$ (schoenite, picromerite)
$K_2Mg(SO_4)_2 \cdot 4H_2O$ (leonite)
$K_2Mg_2(SO_4)_3$ (langbeinite)

Zinc chemistry

ZnS – NaCl – pH dependence
ZnS – NaCl – H_2S – pH dependence
ZnS – NaHS – H_2S
ZnO - KOH, including electrical conductivity

Lead chemistry - revised

PbS – HCl
PbS – NaCl - H_2S – pH dependence
PbS – NaHS – H_2S

Calcium sulfate chemistry - revised

$CaSO_4$ - NaCl

Bromide chemistry

$ZnBr_2$
$CaBr_2$ (revised)
$ZnBr_2$ – $CaBr_2$

Struvite and magnesium phosphate chemistry

Mg – NH_3 – PO_4 system including
$MgNH_4PO_4 \cdot 6H_2O$ (struvite)
$MgHPO_4 \cdot 3H_2O$
$Mg_3(PO_4)_2 \cdot 8H_2O$
$Mg_3(PO_4)_2 \cdot 22H_2O$

Iron chemistry - revised

$FeCl_2$ - HCl

Hydrometallurgical systems - revised

$CaSO_4$ – $ZnSO_4$ – $MgSO_4$ – $MnSO_4$ – Na_2SO_4 – $(NH_4)_2SO_4$ – H_2SO_4
$CaSO_4$ – $NiSO_4$ – $Fe_2(SO_4)_3$ – $MgSO_4$ – $Al_2(SO_4)$ - LiCl – H_2SO_4

Rare earth element chemistry

Estimates for rare earth sulfates including double REE-Na sulfate salts

$Eu_2(SO_4)_3$ – Na_2SO_4
$Tb_2(SO_4)_3$ – Na_2SO_4
$Ho_2(SO_4)_3$ – Na_2SO_4
$Yb_2(SO_4)_3$ – Na_2SO_4
$Lu_2(SO_4)_3$ – Na_2SO_4

Mercaptan systems

Mercaptan - hydrocarbon binaries

Methanethiol – methane, propane, hexane, toluene, decane
Ethanethiol – methane, propane, propylene, butane, pentane, isopentane, hexane, toluene, decane
Propanethiol – butane, pentane, hexane, methylcyclopentane, cyclohexane, toluene
Butanethiol –hexane, methylcyclopentane, heptane, methylcyclohexane, toluene, 2,2,4-trimethyloctane

Mercaptan – water – hydrocarbon - NaOH systems

Mercaptans: methanethiol, ethanethiol, propanethiol, butanethiol, pentanethiol, hexanethiol, heptanethiol
Hydrocarbons: butane, 2,2,4-trimethylpentane; estimates for C1-C10

Amine systems

Diethylenetriamine – H_2O – CO_2
Monomethylethanolamine – H_2O – CO_2

Methanol chemistry - revised $MgSO_4$ – methanol – H_2O Ammonia chemistry - revised

NH_3 – H_2O including transport properties
NH_2Cl – $NHCl_2$ – NCl_3 – NH_3 – Cl_2 – HClO – H_2O
NH_4HS – NH_3 – H_2S – H_2O
Methacrylic acid – NH_3 – ammonium methacrylate
Ni – NH_3
$Fe(OH)_2$ + NH_3 + HCl
$Fe(OH)_2$ + NH_3 + H_2SO_4
NH_4Cl – HCl – NH_3
$NiO/Ni(OH)_2$ + NH_3
$CuO/Cu(OH)_2$ + NH_3 + NaOH
Cu_2O – NH_3
CO_2 + NH_3 + H_2O (including NH_4HCO_3, $(NH_4)_2CO_3$, $NH_4CO_2NH_2$)

Urea + NH_3 + CO_2
NH_3 – methanol
NH_3 – hexane
NH_3 – ethanol
NH_3 – H_2
NH_3 – C_2H_2
NH_2OH – NH_3
NH_3 – NH_4NO_3
NH_3 – $(NH_4)_2SO_4$
NH_4VO_3 – NH_3
$NiSO_4$ – NH_3 – H_2O (including $Ni(NH_3)_5SO_4$)
NH_3 – MoO_3 – H_2O including $(NH_4)_6Mo_8O_{27}.4H_2O$
NH_3 transport properties
NH_3 + K_2CO_3
NH_4HF + NH_3

Miscellaneous

Materials code for elemental hydrogen changed to H(0)
Removing Ti^{4+} as synonym for $Ti(H_2O)_4^{4+}$

GEMSE

$NaCa_2Si_3O_8(OH)$ (pectolite) – moved from MSEPUB

Aqueous databanks:

PUBLIC:

Miscellaneous

Materials code for elemental hydrogen changed to H(0)
Temperature range eliminated for $SrSO_3$

CORROSION KINETICS:

Alloy 2507

Corrosive environments:

NaCl
Seawater
H_2S – NaCl
CO_2 - NaCl
CO_2 – H_2S – NaCl
NaOH
Formic acid
Formic acdi + NaCl
Acetic acid
H_2SO_4

HCl
HNO_3
H_3PO
4
$HCl – H_2SO_4$
$NaCl – H_2SO_4$
$HCl - HNO_3$
$HF – H_3PO_4$
H_2SO_4 –
HNO_3 HF -
HNO_3 H_2SO_4
$FeCl_3 – HCl$
$Fe_2(SO_4)_3 – H_2SO_4 – HCl$
$CuCl_2$ - HCl

Alloy 304 – revision

Repassivation potential parameters in:

$$NaCl – NaF – NaNO_2 – NaNO_3$$

Databank Fixes

Bug Number	Customer Case Number	Description	Reporter	Resolved By
3747	14255	*The PUBLIC databank species SRSO3 has a TRANGE for the solid but no KFIT. The TRANGE IS [-273.15, -273.15] K. Usually this means the solid is to be excluded.* *If so, then we should remove the species or otherwise remove the TRANGE.* Removed temperature range	User (Texas, USA)	ML
4055	14844	*Data for Na2SO4-B(OH)3-K2SO4 is overpredicting solubility* Partially updated as result of potash project	User (Washington, USA)	ML, PW
4757	16413	*FEATURE: Move the species PECTOLITE from MSEPUB to GEMSE* Moved	User (Washington, USA)	ML
4868	16700	*Oxidation state of hydrogen (neutral) is not displayed* Materials code for elemental hydrogen changed to H(0)	User (New Jersey, USA)	ML
4932	16877	*Formula display name for Ti+4 is actually the species Ti(H2O)4+4* Removing Ti4+ as synonym for Ti(H2O)44+	User (New Jersey)	ML
4933	14619	*Kb values and pH difference for the NH3 water system* Massive refit of ammonia data. NH3 – H2O including transport properties NH2Cl – NHCl2 – NCl3 – NH3 – Cl2 – HClO – H2O NH4HS – NH3 – H2S – H2O Methacrylic acid – NH3 – ammonium methacrylate Ni – NH3 Fe(OH)2 + NH3 + HCl Fe(OH)2 + NH3 + H2SO4 NH4Cl – HCl – NH3 NiO/Ni(OH)2 + NH3¬ CuO/Cu(OH)2 + NH3 + NaOH Cu2O – NH3 CO2 + NH3 + H2O (including NH4HCO3, (NH4)2CO3, NH4CO2NH2) Urea + NH3 + CO2 NH3 – methanol NH3 – hexane NH3 – ethanol NH3 – H2 NH3 – C2H2 NH2OH – NH3 NH3 – NH4NO3 NH3 – (NH4)2SO4 NH4VO3 – NH3 NiSO4 – NH3 – H2O (including Ni(NH3)5SO4) NH3 – MoO3 – H2O including (NH4)6Mo8O27.4H2O NH3 transport properties NH3 + K2CO3 NH4HF + NH3	User (Pennsylvania, USA)	RS

Engine/Solver

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
4771		Engine	***When calling CalcRigorousPrescale it crashes occasionally. this was tracked down to the JSOLID array being sized to NI and access using NU.*** The array size was corrected to NU	OLI(CD)	AR
4892		Engine	***Density for Tetracontane (C40H82) at bubble point pressure fluctuates widely for MSE-SRK.*** This happens when pressure calculation in SRK fails and the unconverged pressure is used for further calculation. Volume calculation from SRK is preserved and used directly for those calculation.	OLI(PK)	PK
4893	16792	Security	***BATCH file program returns a security error when it runs*** No security login/logout implemented for espbat program. Added it	User (Japan)	AR
OS-246	17358	Engine	**Make sure bubble point and dew point pressures are realistic and eliminate incorrectly converged results.** Extensive testing to confirm that edge effects are valid	OLI (AR)	AR
OS-270	17078	Engine	***MSE_SRK Assay resulting in Vapor with small or large amount of water, however, the result should be 2nd Liquid. MSE and AQ model results to 2nd liquid.*** Phase edge detection improved	OLI	AR
OS-277	17061	Engine	***Missing INAM and RADI in transport properties chapter are required to calculated crystal radius of complex ions. This will help getting a rough estimate of hydration number. This is both for AQ and MSE model.*** Rather than filling in the INAM and RADI entries for which primary data are not available, it is much more practical to define default values for the hydration numbers according to the regularities observed based on the compilation of Marcus (Ion Properties).	OLI (PK)	PK, A

OLI Studio/Analyzer

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
4887		Framework	***Fugacity Coefficients are reported for the 2nd liquid phase in MSE-SRK. Only fugacities should be reported.***. For SRK, Fugacity Coeff should have 2ndLiq calculated. EqSolver needs to call engine to fined out if SRK is used. Also fixed is that survey never reports 2ndLiq Fugacity Coeff even if it is not MSEH3OION model. Now both survey and single point should report 2ndLiq Fugacity Coeff as long as it is not MSEH3OION.	OLI (CD)	WS

OLI Flowsheet: ESP

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
4213	16522	Chemistry Model	***Flowsheet does not show warnings passed in the WARNING vector (not ERROR vector) during chemistry generation.*** This was a regression introduced with the changes made forBug 4732 (Errors are erased as fixes are made). Corrected the code that caused the regression.	OLI (RN)	SD
4439		User Interface	**Priority List Item: Add RO Membrane UI** Added new RO Membrane unit operation. This was available in version 9.5.4 as a beta item. It is now generally available.	OLI (OLI Development Team)	SD
4451		User Interface	***Priority List Item: Unit Operation - Incinerator*** it is a Gas Incinerator, it has been added	OLI (OLI Development Team)	ZL
4668	16221	User Interface	***UNITS: want to change solid fraction from mole units to mass units (similar vapor to volume units)*** - Added a new volumn fraction unit setting - Reporting Liquid-1, Solid, Vapor, Liquid-2 and Total in the new Phase Fraction section - New section including True, Apparent Mole, Mass, Volume Fraction in all phases	User (Delaware)	ZL
4704	16293	Engine	***The attached cases have one that converges when the number of vessels is set (at 26). The other is essentially the same case but the volume recovery is set and the number of vessels is allowed to adjust. This fails.*** Fixed with current version of the engine as in development build.	OLI (JB)	PK
4719	16326	User Interface	***CONTROLLER: The current requirement for the controller is that both the min and max must be specified. Is this necessary, and is it possible to modify the code so that the user need only set one?*** Showing default values in grey color	User (New Jersey)	ZL
4731	16360	User Interface	***Missing object name for apparent recycle error. Is it possible to link the error message to the set tear streams screen, which is hidden under the process options? A tooltip? Help button?*** Implemented realtime checking for recycles/tear streams. If an error is found, it is reported in the errors window with additional hyperlinked guidance text to launch the tear selection UI.	OLI (RN)	SD

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
4795	16455	User Interface	***KINETICS section. PLEEEEASE label the kinetic variables for the Arrhenius input with units !!!!!!!*** Added units to the captions for keywords for std (arrhenius) rate definition. Also, now displaying a short description for said keywords as a tooltip when mouse hovers over the keyword in the variables definition grid	User (Delaware)	SD
4800		User Interface	***When the equation for a kinetics reaction is modified by clicking on the 'Modify..,' button in the 'Edit Kinetics Reactions' dialog, the modifications are not applied.*** Fixed bug in code that tests to check if the modified kinetics equation is a duplicate of an existing equation.	OLI (SD)	SD
4828		Chemistry Model	***FEATURE: Add MSESRK databank family support*** MSESRK framework support added Added warnings for components (inflows or related inflows) that have not been validated against the MSE-SRK thermo framwork. The warnings are shown in both the chemistry model's inflows grid as well as in the Errors window. To facilitate the above changes, the inflows grid now also displays the related inflows as an additional section. This new section is initially collapsed (or un-expanded) by default.	OLI (OLI Development Team)	ZL
4844	16570	Chemistry Model	***I noticed that when I entered an incorrect Define statement. That the Rate equation disappeared.*** The rate expression was getting reset in the internal data structure when a define variable was added/renamed	User (New Jersey)	SD
4846		User Interface	***1. Add a splitter block or a membrane block, (one input blocks)*** ***2. Connect a stream to the input*** ***3. Go to the properties panel and use the drop down to disconnect the stream*** ***4. Use the drop down again to connect the stream and it does not connect visually***. Disconnecting and subsequently reconnecting an inlet stream from a unit operation's property page was causing the link to remain visually disconnected in the flowsheet. Corrected code that was responsible for re-routing the link.	OLI (RN)	SD

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
4855		User Interface	***When a sensitivity parameter range value edit field has keyboard focus and the simulation is run, the edit field starts behaving erratically.*** ***This happens when the edit control becomes disabled for the duration of the simulation and is automatically re-enabled when the simulation completes. When it re-enables and we click on another field and then back to the original edit field, the edit field does not activate and stops accepting keyboard input in some cases.*** Fixed code that was handling keyboard input events.	OLI (RDY)	SD
4860	16573	User Interface	***When dragging from Studio to ESP, the dragged stream in ESP does not display the default units but go to the program standard (moles...). I could find no way to automatically apply the ESP units to the dragged stream, which means that I need to redefine the units every time I drag a revised stream.*** Improved code to setup units for pasted stream. The program will import the stream in the original source units whenever possible. When the source units are not supported (namely concentration by volume), the program now converts the stream to the process's default units.	User (Montreal, Quebec, Canda)	SD
4885	16780	Chemistry Model	***A user was unable to use the MSE-SRK thermodynamic Framework in the beta test.*** - Corrected SRK database family keyword to match the engine keyword "SRKH3O" - Need to update DataProvider and OLISQLiteDataProvider DLLs - Update OLIDatabaseConverter - Reconvert SRK database	Beta Tester (Australia)	ZL
4891	16789	Error Message	***In ESP original, feedback controller can be used to control composition such as mole fraction in a particular phase. This per phase selection is not there in OLI Flowsheet. So, controlling a composition at one particular phase is difficult for a mixed-phase stream.*** Added code to show phase selection options in the specifications page for a controller when the targeting composition in fraction/concentration units.	OLI(PK)	SD

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
4897		User Interface	***In ESP original, feedback controller can be used to control composition such as mole fraction in a particular phase. This per phase selection is not there in OLI Flowsheet. So, controlling a composition at one particular phase is difficult for a mixed-phase stream.*** Added code to show phase selection options in the specifications page for a controller when the targeting composition in fraction/concentration units.	OLI(PK)	SD
4918	16878	Error Message	***An error occurred while running the simulation. Details: Unspecified run-time error*** The inlet to RO membrane was not connected (it looks to be connected since the stream F-3-5D is touching it but is not actually connected). Added code to check if the all required inlets and outlets to the RO membrane block are connected and report errors in the Errors window.	User (New Jersey, USA)	SD
OS-27	17063	Engine, User Interface	***Currently cross-referencing hydration number calculations for both the models. Hydration number calculation for charged heavy metal complexes seem unrealistic for the AQ model. This may be a limitation of AQ model for dealing with Uranium complexes through membrane***. The rigorous model was extended to have a simpler model when negative values were obtained.	OLI (New Jersey)	PK
OS-36	16761	User Interface	***(RO Membranes) FEATURE: Customer is looking for a membrane manager to be able to view the membrane data and possible see a datasheet.*** Membrane manufacturer data has been incorporated into the source code.	User (Canada)	SD
OS-37	16760	Engine, User Interface	***"THE RATED VESSEL CAN APPROXIMATELY PRODUCE A MAXIMUM PERMEATE FLOW OF 0.65291 M3, AND MINIMUM PERMEATE FLOW OF 0.21546 M3, DEPENDING ON FEED OSMOTIC PRESSURE. INCRESE FEED FLOW RATE OR CHOOSE THE RIGHT SIZE OF MEMBRANE" . Issue no 2 - The message talk about flow, but quotes volume? In the end the error was due to a feed pressure too high: pressure is not even mentioned in the message.*** Proposed verbiage for the changed error message: Based on your settings, the permeate will be between 0.21546 m3/hr and 0.65291 m3/hr. However, your RO-block input feed is only 0.11954 m3/hr. To resolve this error, raise the input feed to at least half-way between the Min and Max values.	Beta Tester (Montreal)	PK

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
OS-38	16738	Engine, User Interface	***have difficulties reading this message on the screen, it is not properly formatted: "THE RATED VESSEL CAN APPROXIMATELY PRODUCE A MAXIMUM PERMEATE FLOW OF 0.65291 M3, AND MINIMUM PERMEATE FLOW OF 0.21546 M3, DEPENDING ON FEED OSMOTIC PRESSURE. INCRESE FEED FLOW RATE OR CHOOSE THE RIGHT SIZE OF MEMBRANE" . Please make sure the message wrap around the Error window, and drop these all caps statements.*** The messages now properly wrap in the error dialog and the font changed to be more readable.	User (Montreal)	SD,PK
OS-40	16733	Engine	**We just had an RO introduction and the end-user asked me about thiosulfate. I added as low as 1ppm Na2S2O3 to my introduction case and it failed with a NAN at the last iteration. If you remove the Na2S2O3, the simulation works fine. Again, I hope it's a simple misuse of the tool on my part.** Case should actually have failed. A singular matrix was created. The error handling routines were updated.	User (Montreal)	PK
OS-68	16879	User Interface	***The H2O Liquid 2 is missing from the list for Species Composition in the Feed forward and Feed Back controllers*** Missing component added to list	User (New Jersey)	CD
OS-225	16799	Engine	***(RO Membranes) The calculations can be extremely sensitive to the feed pressure. The attached simulation ESP2 will fail repeatedly if the pressure is changed by only 5 kPa. The saved version works, but increasing the pressure will cause various failures, either NAN our matrix inversion, it varies. This lack of robustness is problematic.*** For steep slope, steps were damped.	User (Canada)	PK
OS-227	17020	User Interface	***FEATURE: User would like to update an existing stream in OLI Flowsheet to reduce the amount of work needed when pasting a new stream to replace an existing stream in OLI Flowsheet.*** Copy and Paste previously implemented but the copy allows to update an existing stream.	ODT(SD)	SD

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
OS-229	17062	Engine, User Interface	***Please look at the attached RO calculation. This is one of thirty-six RO experiments that Veolia commissioned.*** ***The issue is that several metals, Mg+2, Cu+2, Ni+2, and Pb+2 are have zero permeabilities (rejected completely). I'm focusing on Mg+2 in the callouts.*** ***I've tried doubling the flow rates and pressures, but got the same results.*** Better convergence obtained	OLI (New Jersey)	PK
OS-243	16851	User Interface	***The osmotic pressure is critical to the RO calculation, and presently the user needs to manually adjust the pump (or mixer) outlet pressure so that the RO block doesn't converge because of osmotic-hydraulic differences. The goal is to make something like this be possible – the water's osmotic pressure is fed to the FF and that value plus a differential (perhaps Prodip can suggest the differential P) is forwarded to the pump.*** Enabled controller to measure osmotic pressure	OLI (New Jersey)	AR, ZL
OS-246	17035	Engine	***Three RO Membrane error messages commonly seen on failures and investigating reasons behind it so as to come up with a new verbiage for those error messages.*** Updates/corrections include: 1. Correction in fouling factor calculation 2. Update in membrane calibration convergence, tight tolerance, iteration count, initializing variables 3. Improvement in membrane solver convergence	OLI	PK
OS-249	16930	User Interface	***A user created the attached case and used reaction kinetics for equations from the GeoChem database. These equations have the obsolete keyword "GEN". The equation parser should ignore this keyword.*** The plan for this issue is to remove the GEN keyword from the databanks, it is no longer used the text is completely ignored.	OLI (New Jersey)	CD

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
OS-250	16935	User Interface	***A user currently as a problem in that he needs to have two (or more) chemistry models in a single process. Each model has the same inflows but will use different databases.*** ***What he is trying to simulate is fast reaction kinetics vs. slow reaction kinetics. In one database a species has no equilibrium equation which means the ions are completely dissociated (Fast kinetics). Elsewhere in the process the component has an equilibrium equation (slow kinetics).*** ***Currently you can only specify the databases to be uses in the master model*** Added support for multiple chemistry models to have different databanks provided that they are within the same thermodynamic family	User (Delaware)	SD
OS-255	16955	User Interface	***Missing Stream Parameters (ORP) (also affects controllers)*** Added ORP in the report and allow user to set spec. type to ORP in controller	OLI (New Jersey)	ZL
OS-265	16994	User Interface	***"Solid Only" stream reports a liquid phase when it probably should not*** Added code in Flowsheet: ESP to handle the odd cases where the true speciation data returned from the solver includes non-zero H2O liq-1 phase even though the total liq-1 amount is zero.	OLI (New Jersey)	AR, SD
OS-272	17002	User Interface	***I noticed that the molecular conversion output does not have related inflows. ESP Original has all the related inflows in the Molecular Conversion Option. Case is attached.*** ***The users want to eliminate P2O5 from the apparent output. However due to absence of that option, they can not do that. They only have Ca3PO4 in the inflows and no P2O5.*** Related inflow list has been added to the molecular conversion option	User (Tennessee)	SD
OS-277	17061	Engine	***Missing INAM and RADI in transport properties chapter are required to calculated crystal radius of complex ions. This will help getting a rough estimate of hydration number. This is both for AQ and MSE model.*** Rather than filling in the INAM and RADI entries for which primary data are not available, it is much more practical to define default values for the hydration numbers according to the regularities observed based on the compilation of Marcus (Ion Properties).	OLI (PK)	PK, AA

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
OS-291	17163	User Interface	***(Feature) In order to make the membrane library more useful to customers, Technical Support/Customer Success needs to provide a recommended list of membranes for the library.*** Membrane list created	OLI	WS
OS-303	17162	Engine	***Factoring the membrane area internally when feed flow rate too high or too low for the membrane. Membranes only handle a fixed amount of feed flow for a given membrane area, feed pressure, permeability. Users may not have idea how much the membrane can handle. Having the capability of factoring membrane area internally may help convergence for some cases.*** The algorithm was modified to vary the area for those special conditions. Warning message to display: The simulation cannot be performed with the current settings because the estimated permeate flux is greater than or nearly equal to the calculated feed flow rate to the membrane. The specified element area was reduced by xx% from X m2 to Y m2 to allow the simulation to continue.	OLI	PK
OS-306	17129	User Interface	***FEATURE: From the requirements document. The Extractor block exists in ESP-O but only supports the AQ framework. Engine work would have to be done to allow the Extractor block to work with MSE.*** A development build of Flowsheet: ESP with extractor block was built on 2/6/2018 for developer-level testing. Per discussion with developer team including Bob: 1. Bob tested said development build and fixed several engine related issues that were observed. 2. Bob is going to add reporting of solid phases in the engine results. 3. Said solid phases need to be reported in Flowsheet: ESP's report. 4. The phase for density is incorrectly labeled in Flowsheet: ESP's extractor block's report. This needs to be corrected.	OLI	SD, RDY

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
OS-305	17095	Engine	***Please run the case. It will fail at RO-1, and the error is a negative driving force, with a reported osmotic differential pressure of 32.755 atm (see image).*** ***The RO-1 inlet stream is very dilute, and if you change the booster-1 pressure to 22 atm (it is set to 21 right now), the calculation converges in the first pass, and the calculated osmotic pressure of the concentrate streams (S23 or RO-1 conc) is 2.2 atm. Therefore, the 32.755 atm differential pressure reported in the Error does not appear to be linked to this calculation.*** Updates/corrections: 1. Update error reporting 2. Less failure errors than before due to area factoring work	OLI	PK
OS-311	17378	User Interface	***In the membrane manager, secondary components are usually defined as total dissolved element (e.g., total boron(III) in solution). To avoid confusion between the total dissolved element and a particular species, an explanation needs to be added in the membrane manager.*** Added an additional field to the manufacturer's data record used in the membrane library's underlying database. The additional field can be used to specify an alternate component name for species whose performance data is given. Updated the previously populated excel database file to include the additional field. This field is optional and currently only available for "Species 2" in the database. Manufacture or customers can provide alternate text to display for the 2nd salt. Also fixed is that the top left corner icon is now removed. The grid will show the formula and when mouse is hovering a tooltip will show the display name for the species.	OLI	SD, WS
OS-318	17363	User Interface	***Sometimes multiple callouts need to be placed for different streams but showing essentially the same variables. There is currently no easy way to copy and paste callouts.*** Implemented Callout copy and paste for the following 3 use cases Copy a callout and right click a stream or a block to paste Copy a callout and right click another callout to paste and overwrite the callout Copy a callout and right click an empty location on the flowsheet, pasting with a popup a stream/block dialog after selecting a valid object	OLI	ZL

Bug ID	OLI Case	AREA	Description	Reported by	Resolved by
OS-346	17271	User Interface	***When working with Multiple Chemistry Models, the manipulator block does not correctly map components.*** Inflow species were mapped to use in the block specific chemistry model.	OLI	SD, PK
OS-353	17444	User Interface	***FEATURE: Is it possible to get in the Hide Zero values for the Callout variable table. It would be on by default.*** Hide zero species in variable selection dialog tree node Add a check box to turn on or off (Default ON) Displaying hide zero messages	OLI	ZL

OLI Chemistry Wizard

Bug ID	OLI Case	Alliance Product	Description	Reported by	Resolved by
4571	15900	ProII	***Assays and PC, Units of Measure do not display correctly on Korean or Japanese windows*** Added code to correctly translate degree symbol on foreign OS.	Schneider Electric	CD
4826		ALL	***FEATURE: Add support for new MSE-SRK Thermodynamic Framework*** Added support for MSE-SRK Thermodynamic Framework	OLI (CD)	CD
4850		Aspen Plus	***The tickbox on the last screen of Chemistry Wizard for AspenPlus Component ID and Alias for components with errors does not refresh the screen. User needs to go back one screen and click next in order to see the components with error message if any.*** When the grid was updated for 9.5 the connection from the check box to the event was deleted. Reconnected the event.	OLI (CD)	CD
4882		ALL	***The new MSE+SRK databank family needs to be implemented in OLI ChemistryWizard*** Added support for MSE-SRK Warnings are shown at the summary screen. When the switch is made to unified databanks we need to add ui warnings like OLI Studio.	OLI(CD)	CD
4903		ALL	***Available and selected databank lists do not scroll horizontally to show entire name*** Added code to show scroll bars when necessary and also made lists a little wider	OLI(CD)	CD
OS-355	17442	ALL	***Previously Chemistry wizard relied on the generator to fail cases when security was no passing for MSE. Chemistry Wizard is now security enabled so it should check.*** Added SRK and MSE serial number security check. If the framework is not enabled in a serial number, it will not be shown in the drop-down option	OLI	ZL

OLI Alliance Products

General Notes for the alliance products:

There were no major upgrades to the alliance products for 9.6.1. There were some specific upgrades for each alliance product.